Stability of Nagaoka phase, spin effective action and delocalized free holes

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Abstract

The Hubbard model in the limit of infinite U is investigated within a projected slave fermion representation and following a previous work of the author and collaborators [1]. The stability of the Nagaoka's phase with respect to a non vanishing concentration of holes (δ_h) is analyzed by envisaging the existence of a spin effective action for itinerant magnetism of the Hubbard model. It is considered that, as the hole doping increases away from the half filled insulating limit, free holes are expected to be more delocalized. Depending on treatment for the hopping: a ferromagnetic or anti-ferromagnetic ordering might arise and the Nagaoka phase might have some stability with respect to $\delta_h \neq 0$.

Key words: Strong correlations, Nagaoka phase, concentration of holes, Hubbard model, hopping, spin effective action

1. Introduction

One of the few exact results for the Hubbard model (HM) is the ferromagnetic Nagaoka limit for $U = \infty$ [2,3]. This phase appears when one hole hops in the half filled band. Although this limit is not found in any material, it can be reached in optical traps [4]. The investigation of the Nagaoka mechanism provides relevant information about the phase diagram of the model and one starting point for understanding further the role of strong electronic correlations [1,5,6,7] and of realistic mechanism for itinerant (ferro)magnetism [5,3]. In the limit of infinite Coulomb repulsion the HM is written as:

$$H = -\sum_{ij,\sigma} t_{ij} \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \mu \sum_{i\sigma} (1 - \tilde{c}^\dagger_{i\sigma} \tilde{c}_{i\sigma}),$$

where t_{ij} is a symmetric matrix with elements representing the hopping amplitude t only non-zero between the nearest-neighbor sites; $\tilde{c}_{i\sigma}$ is the projected electronic operator [5]. In this expression the chemical potential μ is to control the number of vacancies (away from half filling), and the projected electronic operator carries the effect of the strong correlations, i.e. it excludes the doubly occupied states.

It is difficult to handle the strong electronic correlations and thus to provide exact results, in particular concerning the stability of the Nagaoka phase. However, a common trend is that this FM phase is unstable with respect to a finite concentration of holes in particular in the thermodynamic limit [8,9,10,11,12,13,14]. In the present work we investigate the role of the delocalization of (free) holes for the appearance and for the stability of the Nagaoka's phase following the long-wavelength approach with slave fermion representation worked out in Ref. [1]. By envisaging the derivation of a spin-effective action (S_{eff}) for the HM with very large U, a previous analysis was performed in Ref. [1]. On the other hand, in the present work, the role of delocalization of free holes close to half filling is investigated. It is considered that the increase of the number or concentration of holes should increase the mobility of holes departing from the half filled limit. An itinerant magnetic phase (ferromagnetic or anti-ferromagnetic) emerges depending on the structure and treatment of the hopping of spinless holes.

2. Slave fermion for the $U = \infty$ Hubbard model

To account for the strong correlations that forbid doubly occupied states, consider the slave-fermion decomposition for projected electronic operators [16] given by: $\tilde{c}^\dagger_{i\sigma} = b^\dagger_{i\sigma} f_i$, where two operators have been used: $b_{i\sigma}$ stands for a spinon boson and $f^\dagger_i$ creates a charged spinless fermion. The functional generator for the $U = \infty$ Hubbard model is given by: $Z_{U=\infty} = \int \mathcal{D}[b, b^\dagger; f, f^\dagger] \exp\left(S^{SF}_{U=\infty}[b_i, b^\dagger_i; f_i, f^\dagger_i]\right)$. The action can be written, with the time-dependent phase, as [1]:

$$S^{SF}_{U=\infty} = -\int d\tau \sum_{<i,j>} f_i \left[(\partial_\tau + \mu)\, \delta_{ij} + \sum_\sigma t_{ij} b^\dagger_{i\sigma} b_{j\sigma} \right] f^\dagger_j$$

$$-\int d\tau \sum_i \left(\sum_\sigma \; b^\dagger_{i\sigma}\partial_\tau b_{i\sigma} - H_{constr} \right) \qquad (1)$$

The local non doubly occupancy (NDO) constraint is imposed by a (local) Lagrange multiplier, λ_i, by adding the term: $H_{constr} = \lambda_i (f_i^\dagger f_i + \sum_{\sigma=\uparrow,\downarrow} \; b^\dagger_{i\sigma} b_{i\sigma} - 1)$.

The slave-fermion decomposition is equivalent to a particular (lowest weight) representation of the $su(2|1)$ supersymmetric projected electronic operators [6,17]: spinless holes are super-partners of spinons. A mapping for the variables, incorporating implicitly the non-doubly-occupancy (NDO) constraint, is given by [1]:

$$(b_{i\uparrow}, \quad b_{i\downarrow}, \quad f_i) = \frac{(e^{i\phi_i}, \quad z_i e^{i\phi_i}, \quad \xi_i e^{i\phi_i})}{\sqrt{1+\overline{z}_i z_i + \overline{\xi}_i \xi_i}}, \qquad (2)$$

and the corresponding variables for $b^\dagger_{i,\sigma}$ and $f^\dagger_i$. With these new variables (z_i, ξ_i, ϕ_i respectively for bosonic spinons, spinless fermions and a local phase) the Lagrange multiplier λ_i is eliminated naturally, being the NDO constraint incorporated. With the spinon variables z_i, the images of the spin $su(2)$ algebra - $\vec{S}$ - can be rewritten [1,17], for example: $S^{cl}_z = \frac{1}{2}\frac{1-|z|^2}{1+|z|^2}$. There is a local gauge invariance as consequence of the redundancy in parameterization of the electron operator in terms of the auxiliary boson/fermion fields. After some manipulation, decomposing the measure of the path integral into the new variables $\mathcal{D}[b,b^\dagger;f,f^\dagger] \to D\mu_{spin}(\overline{z},z) \times D\mu_{fermion}(\overline{\xi},\xi)$, with the corresponding Jacobian [17], the action reads [17,1]:

$$S = \sum_i \int_0^\beta ia_i(\tau)d\tau - \sum_i \int_0^\beta \bar{\xi}_i \left(\partial_\tau + \mu + ia_i\right)\xi_i d\tau$$
$$- \int_0^\beta t \sum_{ij} (\overline{\xi}_j \xi_i < z_i|z_j > + hc)\, d\tau \qquad (3)$$

The first term of this action is a kinematical term and the second is the classical image of the Hamiltonian. The spin "kinetic" term (Berry phase): $ia = - < z|\partial_t|z >= \frac{1}{2}\frac{\dot{\bar{z}}z - \bar{z}\dot{z}}{1+|z|^2}$, with $|z\rangle$ being the su(2) coherent state [17,1]. The inner product of the su(2) coherent states is written as: $\langle z_i|z_j\rangle = \frac{1+\overline{z}_i z_j}{\sqrt{(1+|z_j|^2)(1+|z_i|^2)}} \equiv \frac{1}{t_{ij}}\Sigma_{ij}$.

3. Factorization of the hopping

By introducing more holes in the half filled HM, it can be expected they become progressively more delocalized. Consider that the band structure is such that the hopping term can be decomposed into two parts. One of them endows the holes with a dispersion relation (labeled by γ_1) and the other is treated as a perturbation (labeled by γ_2), eventually from a different band. It will be considered schematically that:

$$\bar{\xi}_i \Sigma_{ij} \xi_j \to \gamma_1 \; \bar{\xi}^{(1)}_j \xi^{(1)}_i \Sigma^{(1)}_{ij} + \gamma_2 \; \bar{\xi}^{(2)}_j \xi^{(2)}_i \Sigma^{(2)}_{ij} + h.c. \qquad (4)$$

Where γ_1 and γ_2 keep track of each of the different parts of the hopping. The procedure and idea will be clearer and useful when working in the momentum space. We will consider that these terms are characterized by different ranges of momenta of holes $\xi^{(1)}(\mathbf{k}_1)$ and $\xi^{(2)}(\mathbf{k}_2)$, associated respectively to the terms $\Sigma^{(1)}$ and $\Sigma^{(2)}$, such that $\mathbf{k}_1$ and $\mathbf{k}_2$ can belong to different parts of the band. With this decomposition, the following ansatz for the free hole Green's functions can be envisaged:

$$(G_0^{-1})_{ij} = (\partial_\tau - \mu)\,\delta_{ij}\delta(\tau) + \gamma_1 \Sigma^{(1)}{}_{ij}, \qquad (5)$$

and $\gamma_2.\Sigma^{(2)} = \gamma_2 t^{(2)}_{ij} < z_i|z_j >^{(2)}$ is a perturbation. The upper indices $^{(2)}$ stand for the perturbation due to the corresponding part of the hopping term, separated according to expression (4). Since this separation is generic and not calculated microscopicaly, for the sake of generality we can have $t^{(2)}_{ij} \neq t^{(1)}_{ij}$ depending on the hopping (and band) structure. This procedure can be considered such as to provide a measure of the (de)localization of the free holes. For instance, in a normal conducting phase, we should recover $\gamma_2 \to 0$, that is used in the usual mean field approximation [15,1]. On the other hand, at the half filling limit (and very close to it) the hopping parameter would be such that $\gamma_1 = 0$, suitable for the hopping (loop) expansion as discussed in details in Ref. [1].

3.1. *Delocalization of free holes and spin effective action*

We take a continuum limit of the full action, given by (3), to derive a spin-effective action, S_{eff}, by integrating out the fermion variables with the prescription (5) in the same lines as it was done in Ref. [1]. Using a finite difference method for the term labeled by γ_1, we take: $\xi_{j=i+1} \to \tilde{\xi}(i) + a\nabla\tilde{\xi}(i)$ and perform a Fourier transformation. Therefore we consider free holes are endowed with a dispersion relation $\epsilon(\mathbf{k}_{(1)})$, being that $\mathbf{k}_1$ ($\mathbf{k}_2$)refers to the momenta of modes labeled by $\gamma_1(\gamma_2)$. This yields the momentum dependent Green's function: $G_0[\mu;\epsilon(\mathbf{k}^{(1)})]$. The particular dispersion relation $\epsilon(\mathbf{k}^{(1)})$ is completely defined by the lattice (geometry and dimensionality). For the sake of the main argument, we consider a two dimensional square lattice, for which it follows: $\epsilon(\mathbf{k_{(1)}}) \simeq 2\gamma_{(1)} t \sum_{k,\sigma} \; \phi^2_{k,\sigma}\,(cos(k_x) + cos(k_y))$, from what the continuum limit is extracted. Prescription (4) might also be associated to a superposition of (nearly) localized and (fully) delocalized states. In order simplify the notation $\mathbf{k}_{(1)}$ momenta will be denoted simply by $\mathbf{k}$ from here on.

The corresponding effective action, with the integration of fermions variables, can be written as [1]:

$$S_{eff} = Tr\text{Log}G^{-1} \equiv Tr\text{Log}\left(G_0^{-1} - ia + \Sigma^{(2)}\right)$$
$$= Tr\text{Log}G_0^{-1} + Tr\text{Log}(1 - G_0 ia + G_0\Sigma^{(2)}). \qquad (6)$$

The different modes of the fermions are decoupled such that the corresponding $\Sigma^{(i)}$ are treated (nearly) independently. The free hole Green's function can be calculated,

for the sake of generality, for a given (sub)lattice A, instead of an unique lattice, being written as: $(G_0^{-1})^A(\mu^A, \mathbf{k}) = (\partial_\tau - \mu^A + \epsilon_A(\mathbf{k}))^{-1}\delta(\tau)$. This case of (at least) two sublattices will not be worked out here, and this might be considered when there are different hoppings in the sublattices or between each of them. This can yield the terms labeled by γ_1 and γ_2 contributing in each of the different sublattice. The long-wavelength expansion is done by considering $G_0^{-1} >> \Sigma^{(2)}$. The reliability of this expansion depends on several parameters, seen in expressions (4) and (5). Basically it is required that $\mu + \epsilon(\mathbf{k}) >> \Sigma^{(2)}$ where $\Sigma^{(2)}$ is only part of the full hopping term. We remind further that $\Sigma^{(2)}$ is basically proportional to t and the long-wavelength limit corresponds to a gradient expansion of $t < z_i|z_j >$. Therefore we expect to provide a complementary investigation to the loop expansion analyzed in Ref. [1]. considering the role of the delocalization of free holes. For the sake of the argument and to show preliminary analytical results, $\Sigma^{(1)}$ and $\Sigma^{(2)}$ are considered to somehow decouple from each other. In this case the expression for the leading terms of the effective action, is obtained in the very same way as shown in Ref.[1]. Keeping track of the time ordering in the path integral with a Taylor expansion in fluctuating times [18,1], for D-dimensions S_{eff} is given by:

$$\mathcal{S}_{eff} = \int \frac{d^D\mathbf{k}}{(2\pi)^D} \mathrm{Log}\left(1 + exp\left(-\beta(\mu - \epsilon(\mathbf{k}))\right)\right) - \sum_{<i,j>} \int_0^\beta \frac{J_{eff}}{2} | < z_i|z_j > |^2 d\eta - \sum_i \int_0^\beta d\eta K_{eff}\; i\; a_0(\eta) + ... \tag{7}$$

where ... stands for the higher order terms. In the case the spinon dynamics decouples completely from the holes, we rewrite S_{eff} in the momentum space, with zero momentum transfer between holes and spinons. The effective coefficients J_{eff} and K_{eff} can be written as:

$$J_{eff} = -\gamma_2^2 \int_{K_0}^{K_1} \frac{d^D\mathbf{k}}{(2\pi)^D} \frac{t^2\beta}{4cosh^2\left(\frac{\beta(\mu-\epsilon(\mathbf{k}))}{2}\right)} \tag{8}$$

$$K_{eff} = -\int_{K_0}^{K_1} \frac{d^D\mathbf{k}}{(2\pi)^D} \frac{2}{\left(e^{(\beta(\mu-\epsilon(\mathbf{k})))} + 1\right)}. \tag{9}$$

The K_{eff} is the coefficient of the time dependent term and it will not be analyzed here, since it does not modify the magnetic ordering in a first analysis. K_0 and K_1 are the (upper and lower) limiting values of the momenta of holes which contribute in that part of the decomposition of the variables, i.e. holes from γ_1 term. For $\gamma_1 = 0$, the expressions obtained in Ref.[1] are reproduced. In this expression the second order (leading) term can be written in the form of a Heisenberg coupling (either in k-space or in the lattice) as:

$$H_{eff}^{cl} = \frac{J_{eff}}{2} \sum_{(ij)} |\langle z_i|z_j\rangle|^2 = J_{eff} \sum_{(ij)} (\vec{S}_i\vec{S}_j + \frac{1}{4}),$$

where the classical symbols of the spin operators for the quantum $s = 1/2$ Heisenberg model were used [1], and the corresponding modes $\mathbf{k}_1$ and $\mathbf{k}_2$ have been separated. Below we show some expressions for the coefficient of the Heisenberg spin-coupling J_{eff}. The second order term in the effective action (7) has different signs and structures for J_{eff} depending on the range of the parameters. However it is worth emphasizing that due to this separation, the spinon connection ($< z_i|z_j >$) in expression (7) corresponds to only part of the full spinon dynamics (that from $\Sigma^{(2)}$), and therefore the resulting phase might not have a fully saturated (ferro)magnetic ordering. The separation of the full hopping in ranges of momenta, labeled by γ_1, γ_2, is a relevant assumption for this analysis. A cutoff in the momentum integration might correspond to the emergence of a kind of Fermi surface for the vacancies in which an integration in k is limited by k_F, the momentum of holes at the (eventual) Fermi surface. A decomposition in low and high energy modes suggests a renormalization group analysis, which will be presented elsewhere. However separation of modes has been also implemented in, for example, Ref. [19].

3.2. *Some analytical expressions for J_{eff}*

The particular dispersion relation for the holes was not explicitly written so far. For the sake of generality, two cases are considered of the following usual forms: $\epsilon_{(I)}(\mathbf{k}) = \gamma_1\tilde{a}_1 k \equiv a_1 k$ and $\epsilon_{(II)}(\mathbf{k}) = \gamma_1\tilde{b}_1\mathbf{k}^2 \equiv b_1\mathbf{k}^2$.

Changing variables for each of the cases, we write:

$$J_{eff}^{(I)} = \gamma_2^2 \frac{2t^2\Omega_D\beta}{4(2\pi)^D\beta a_1} \int_{X_0^{(I)}}^{X_1^{(I)}} d\,x\, \frac{\left[\left(\mu - \frac{2x}{\beta}\right)\frac{1}{a_1}\right]^{D-1}}{cosh^2(x)} \tag{10}$$

$$J_{eff}^{(II)} = \gamma_2^2 \frac{2t^2\Omega_D\beta}{4(2\pi)^D b_1\beta} \int_{X_0^{II}}^{X_1^{(II)}} d\,x\, x \frac{\left[\left(\mu - \frac{2x^2}{\beta}\right)\frac{1}{b_1}\right]^{D-2}}{cosh^2(x)}, \tag{11}$$

where Ω_D is the integral of the D dimensional solid angle; and the cutoffs are: $X_0^{(I)} = \frac{(\mu - a_1K_0)\beta}{2}$, $X_1^{(I)} = \frac{(\mu - a_1K_1)\beta}{2}$, and $X_0^{(II)} = \frac{(\mu - b_1K_0^2)\beta}{2}$, $X_1^{(II)} = \frac{(\mu - b_1K_1^2)\beta}{2}$. With the eventual formation of a Fermi surface for the (spinless) vacancies in a normal metallic phase, we could identify the chemical potential to: $\mu = \epsilon(\mathbf{k}_F)$, where $\mathbf{k}_F$ is the momentum at the Fermi surface. The result for the quadratic $\epsilon_{(II)}$ in 2-dim is the same as for $\epsilon_{(I)}$ in 1-dim, apart from a normalization.

The integrations, in 2 dim, yield respectively:

$$J_{eff}^{(I),D=2} = -\gamma_2^2 \frac{t^2}{4\pi a_1\beta}\left[X_1^{(I)}tanh(X_1^{(I)}) - X_0^{(I)}tanh(X_0^{(I)}) + \frac{2}{\beta}\mathrm{Log}\left(\frac{coshX_1^{(I)}}{coshX_0^{(I)}}\right)\right] \tag{12}$$

$$J_{eff}^{(II),D=2} = \gamma_2^2 \frac{t^2}{4\pi b_1}\left[tanh\left(X_1^{(II)}\right) - tanh(X_0^{(II)})\right] \tag{13}$$

A short example can be taken, for $T = 0$, by choosing $K_1 > K_0 \simeq k_F \simeq \mu/a_1$ for the first of these expressions, in which case K_0 might be the momentum at a Fermi surface for the holes. The resulting spin-effective coupling at zero temperature is given by: $J^{(I)}_{eff} \simeq \gamma_2^2 t^2 (2a_1K_1 - \mu)/(4\pi a_1) > 0$. This is a ferromagnetic coupling representing a Nagaoka-type phase, with some stability since it remains finite for a finite corresponding concentration of holes $\delta_h > 0$. In particular, for very small δ_h, we have the compressibility of holes, $\kappa_h(T \to 0) \to 0$. It is interesting to notice that δ_h and κ_h are calculated analytically. As temperature increases the decay to a paramagnetic phase should take place, depending strongly on the spinon dynamics whose investigation is outside the scope of the present work. We emphasize that the present work only aim to provide a different starting point for investigating the role of delocalization of holes. The appearance of the ferromagnetic coupling however was related to the range of integration of the momenta of holes. Should we consider a different physical picture in which the relation among the variables K_0, K_1, μ were related differently, it can give rise to an (itinerant) anti-ferromagnetic coupling. This analysis remains valid for $U < \infty$.

In the limit of no limitation on the momenta of holes, i.e. $K_0 = 0$ and $K_1 \to \infty$, in 2 dim, it yields respectively:

$$J^{I,D=2}_{eff} \to -\gamma_2^2 t^2 \frac{\mu}{a_1^2\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k}{\sqrt{2k+1}} - \frac{2}{\pi a_1^2 \beta}(Ln2) \qquad (14)$$

$$J^{II,D=2}_{eff} \to -\gamma_2^2 \frac{t^2}{\pi b_1} \sum_{k=0}^{\infty} \frac{(-1)^k}{\sqrt{2k+1}}. \qquad (15)$$

We notice that these couplings might depend on μ. They provide anti-ferromagnetic spin Heisenberg couplings.

4. Final remarks

We have shown that the delocalization of free holes might be a relevant issue for the understanding of the stability of the Nagaoka's phase with respect to a finite concentration of holes. More generally we proposed a framework for investigating different magnetic orderings in the limit of very large Coulomb repulsion and low concentration of holes for the Hubbard model. A spin effective action was found to have a form of localized Heisenberg coupling in the long wavelength limit along with the work presented in Ref. [1]. It can be ferromagnetic (Nagaoka-type phase) or anti-ferromagnetic depending on the relation among the chemical potential and the eventual values of the limitation on the summation/integration of momenta carried by the holes. For that, the hopping term was separated in two parts, corresponding to high and low momentum modes or to hopping among different bands [1]. A microscopic derivation of the prescriptions adopted was not yet presented and for the sake of the main argument it was considered that the holes are reasonably decoupled from the spinons. In particular, by endowing holes with a dispersion relation such that a kind of Fermi surface can be formed, it was found that the Nagaoka's phase at finite concentration of holes can have some stability in a long-wavelength limit. A more complete analysis will be presented elsewhere.

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[1] Eventually the parameters γ_i introduced to label $\Sigma^{(i)}$ might be expected to depend on the temperature, U and concentration of holes δ_h [20,21] becoming phenomenological. For example, one might want to account the variation of γ_i due to a finite value for the Coulomb repulsion by means of prescriptions. They might be given by:

$$(i) \quad \gamma_1 = \frac{\alpha_0}{\alpha_0 + \alpha_U U}, \quad \gamma_2 = \frac{\alpha_U\, U}{\alpha_0 + \alpha_U U},$$
$$(ii) \quad \gamma_1 = \frac{2\alpha_1 + \alpha_2\, U}{2(\alpha_1 + \alpha_U U)}, \quad \gamma_2 = \frac{\alpha_3\, U}{2(\alpha_1 + \alpha_U U)}, \qquad (16)$$

where α_i $(i = 0, U, 1, 2)$ depend on the parameters of the model and their values are bounded by 0 and 1. The values of such parameters must be constrained due to expression (4). For example for this second parameterization, $\alpha_2 + \alpha_3 = 2\alpha_U$. This makes possible to consider that the hopping term contributes both in Σ and in G_0 , whereas in the first prescription (i) we recover the development of Ref. [1], for which $\gamma_1 = 0$ when $U = \infty$.

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